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Seattle, WA 98124-2207

## Final Technical Report

February 1999


Document D6-82405

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# Algorithmic Research and Software Development for an Industrial Strength Sparse Matrix Library for Parallel Computers

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The Contractor, The Boeing Company, hereby certifies that to the best of its knowledge and belief, the technical data delivered herewith under Contract No. DABT63-95-C-0122 is complete, accurate, and complies with all requirement of the contract.

  
\_\_\_\_\_  
Program Manager (or Designee)

2/25/99  
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Date

Prepared for:  
Directorate of Contracting  
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Sponsored by:  
Defense Advanced Research Projects Agency  
ITO (Attn: G. Koob)  
3701 N. Fairfax Drive  
Arlington, VA 22203-1714

Contract: DABT63-95-C-0122  
CDRL A001

PR&C: HJ1500-5212-0677  
AAP No: DAR5 C999

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19990303 052

DTIC QUALITY INSPECTED 1

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public report burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE  01 1999		3. REPORT TYPE AND DATES COVERED  Final Report, September 1995-January 1999
4. TITLE AND SUBTITLE  Algorithmic Research And Software Development For An Industrial Strength Sparse Matrix Library For Parallel Computers			5. FUNDING NUMBERS  (C) DABT63-95-C-0122	
6. AUTHOR(S) Roger G. Grimes				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) The Boeing Company, P.O. Box 3707, M/C 7L-22, Seattle, WA 98124-2207			8. PERFORMING ORGANIZATION REPORT NUMBER  D6-82405	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)  DARPA(ITO) (G. Koob), 3701 N. Fairfax Drive, Arlington, VA 22203-1714 ATZS-DKO-I (J. Bourne), P.O. Box 12748, Ft Huachuca, AZ 85670-2748			10. SPONSORING/MONITORING AGENCY REPORT NUMBER DAR5 C999 CDRL A001	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT  Approved for public release; distribution is unlimited. Requests for this document shall be referred to ATZS-DKO-I (J. Bourne), P.O. Box 12748, Ft Huachuca, AZ 85670-2748			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)  This final report describes the status of work performed during the months of Sept 1995 through Jan 1999 on the Algorithmic Research And Software Development For An Industrial Strength Sparse Matrix Library For Parallel Computers. The objective of this effort was to: 1. Research and demonstrate new algorithms for the solution of systems of linear equations in parallel. 2. Research and demonstrate a new parallel approach for the real symmetric sparse generalized eigenvalue problem.				
14. SUBJECT TERMS Sparse linear algebra, parallel computing			15. NUMBER OF PAGES  3	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT  Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE  Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT  Unclassified	20. LIMITATION OF ABSTRACT  Unlimited	

## **FORWARD**

This Final Report, prepared by The Boeing Company Mathematics and Computing Technology organization, is provided under a Department of Defense contract for research entitled "Algorithmic Research and Software Development for an Industrial Strength Sparse Matrix Library for Parallel Computers". The reporting period is from September 1995 to December 1998. The Defense Advanced Research Projects Agency provided funding under Contract No. DABT63-95-C-0122. Drs. Robert Lucas, Federica Darema, and Gary Koob, DARPA/ITO managed the program for DARPA.

## ABSTRACT

The objective of the effort was to build a parallel sparse matrix library that is needed by applications migrating to parallel computers. Research on robust algorithms for industrial problems and software development for a robust implementation for industrial users are both needed for a sparse matrix library in order for parallel computers to realize their potential to out-perform previous single-threaded hardware and software platforms. An additional challenge faced during the effort was to develop software that would run efficiently on a variety of parallel computers, including both shared memory and distributed memory computers. The effort included work on the solution of sparse systems of linear equations in parallel and work on computing some eigenvalues for sparse real symmetric generalized eigenvalue problems. These technology areas are key for the migration of industrial applications such as Finite Element Analysis to parallel computers.

The effort included new and innovative research on parallel methods for solution of sparse systems of linear equations. A software package, Sparse Object Oriented Linear Equation Solver (SPOOLES), containing all of the developed software for solving real and complex system using both direct and iterative methods for serial, shared memory, and distributed memory computers is now available in the public domain via <http://www.netlib.org/linalg/spooles/spooles.html>.

A parallel eigensolver for parallel computers was also developed and successfully demonstrated on several test problems across a range of computers (Sun, SGI, and HP). Although the amount of code that was actually parallelized is substantial, it is not sufficient to replace the serial implementation in Fortran. In addition, the parallel eigensolver developed during the effort requires that much of the data be replicated on each processor instead of being fully distributed. This leads to significant limitations on problem size capacity, which in turn limits the applicability of the software. Further code development is therefore required for a sparse real symmetric generalized parallel eigensolver that can be used by application programs such as NASTRAN and ANSYS.

## KEY WORDS

sparse linear algebra  
parallel computing  
direct solution  
iterative solution  
eigenvalue  
eigensolver

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## **ACRONYMS, ABBREVIATIONS AND SYMBOLS**

DARPA	Defense Advanced Research Programs Agency
SPOOLES	Sparse Object Oriented Linear Equation Solver

## 1.0 SUMMARY

The Algorithmic Research and Software Development for an Industrial Strength Sparse Matrix Library for Parallel Computers performed algorithmic research on issues associated with the parallel solution of sparse systems of linear equations. We developed a new set of sparse matrix ordering algorithms to both preserve sparsity for the numerical factorization, preserve locality for efficient local computation and to reduce communication and enhance opportunities for parallel computations. We implemented a suite of tools for the direct solution of sparse systems of linear equations supporting both real and complex matrices, both symmetric and unsymmetric systems, and providing pivoting for numerical stability. Based on the direct solution capabilities, we built a drop tolerance incomplete factorization and a suite of iterative methods to complement the direct solution capabilities. We also developed a capability for the parallel solution of large least squares problems.

We also performed research work and preliminary software development for a parallel real sparse generalized eigensolver. While leveraging off our existing serial eigensolver was a viable approach, converting the serial eigensolver to the parallel computing environment was significantly more difficult than originally contemplated, and the developed software requires further research and development to improve both its reliability and parallel efficiency.

## 2.0 INTRODUCTION

The Computational Mathematics staff of the Applied Research and Technology Division of Boeing Shared Services Group is responsible for mathematical software libraries used throughout The Boeing Company. This staff is also responsible for the commercially available software, BCSLIB-EXT, which is used extensively inside and outside of Boeing. In particular, it has become the software of choice for solving large sparse linear algebra equations arising in application areas such as finite element analysis. The Algorithmic Research and Software Development for an Industrial Strength Sparse Matrix Library for Parallel Computers contract sought to develop the basic technology for such a library for parallel computers and to make that technology available to those applications attempting to migrate to parallel computers. The lack of this enabling software technology has been a large stumbling block for the wide spread use of parallel computers for large-scale applications.

The solution of sparse linear algebra problems in parallel has been an active area of research since the advent of parallel computers. However none of this research has produced a viable suite of software for the parallel solution of linear equations that meets the needs of industrial applications.

This suite of software is required to extend the applicability of parallel computers to general use for application areas that have to solve sparse linear algebra problems such as finite element analysis. This contract was an attempt to meet this need.

### **3.0 METHODS, ASSUMPTIONS, AND PROCEDURES**

The research in this contract drew upon Boeing's experience supporting a commercial software library in this application area and knowledge of parallel sparse linear algebra. We identified the key research areas that required breakthroughs before a reliable industrial strength sparse matrix package could be developed. These areas were ordering methods, pivoting for numerical stability, and a robust and reliable direct factorization approach that would work well in serial, shared memory, and distributed memory parallel computing environments.

We selected a development environment using the C language, with POSIX threads for the shared memory computing paradigm and MPI for the distributed memory computing paradigm. We discussed interface issues with technical representatives from computing hardware vendors and leading providers of engineering analysis application packages that were target end users of the results of the contract.

We enlisted the services of Dr. Joseph W. H. Liu, York University, to assist in the first task, which was the development of a new ordering methodology for the direct solution of sparse systems of linear equations.

Our starting point for the parallel eigensolver was the block shift and invert Lanczos software found in BCSLIB-EXT.

### **4.0 RESULTS AND DISCUSSION**

During the course of this contract we have developed a robust and reliable software package, SPOOLES, for the solution of sparse systems of linear equations which include the following features:

- Supports both Real and complex sparse matrices
- Solves systems that are Symmetric, unsymmetric, Hermitian, or overdetermined
- Provides pivoting for numerical stability
- Direct and iterative solution methods
- Available on serial, shared memory parallel, and distributed memory parallel computers

SPOOLES is available in the public domain via NETLIB, a numerical computing software repository at Oak Ridge National Laboratory. Both source code and documentation for SPOOLES is available on the World Wide Web via [www.netlib.org/linalg/spooles/spooles.2.2.html](http://www.netlib.org/linalg/spooles/spooles.2.2.html).

The sparse eigensolver developed during this research program requires further research and software development before it can be used on a widespread basis as a sparse real symmetric generalized parallel eigensolver. Boeing is pursuing additional funding from alternate sources to complete this work.



## 5.0 RECOMMENDATIONS

We recommend that any application developer interested in solving sparse systems of linear equations examine the SPOOLES package for their use.

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) DARPA(ITO) (G. Koob), ATZS-DKO-I (J. Bourne), P.O. Box 12748, Ft Huachuca, AZ 85670-2748			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES  Export Control Restrictions Apply				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Distribution authorized to U.S. Government Agencies and U.S. DoD contractors only; critical technologies. Other requests for this document shall be referred to ATZS-DKO-I (J. Bourne), P.O. Box 12748, Ft Huachuca, AZ 85670-2748			12b. DISTRIBUTION CODE	
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14. SUBJECT TERMS survivable, composite structures, fighter wing, decoupling, fuel containing structure, hydrodynamic ram, cellular structure, cellular wing, tubular structure, tubular wing			15. NUMBER OF PAGES  xx	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT  Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE  Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT  Unclassified	20. LIMITATION OF ABSTRACT  Unlimited	